organic compounds

Ammonium hexafluoridophosphate–18-crown-6 (1/1)

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In the crystal structure of the title compound, $NH_4^+ \cdot PF_6^- \cdot C_{12}H_{24}O_6$, the cation is situated in the 18-crown-6 ring, forming a supramolecular rotator-stator-like structure held by N—H···O hydrogen bonds. The six O atoms of the crown ether lie approximately in a plane [mean deviation 0.2129 (3) Å]; the N atom is displaced by 0.864 (3)Å from the centroid of the 18-crown-6 ring. The slightly distorted tetrahedral cations further interact with the slightly distorted octahedral anions via intermolecular N—H···F hydrogen bonds.

Related literature

For background to 18-crown-6 compounds, see: Bajaj & Poonia (1988); Fender *et al.* (2002); Kryatova *et al.* (2004). For related structures. see: Dapporto *et al.* (1996); Pears *et al.* (1988).
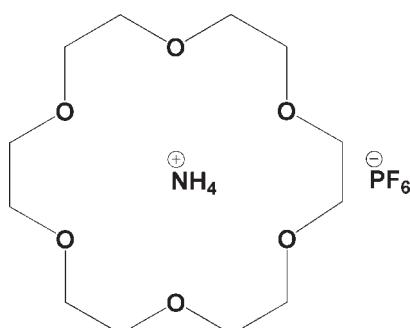
Experimental

Crystal data

$NH_4^+ \cdot PF_6^- \cdot C_{12}H_{24}O_6$
M_r = 427.32
Monoclinic, $P2_1/n$
a = 12.559 (3) Å
b = 8.7352 (17) Å
c = 18.6511 (17) Å
β = 94.097 (10)°
V = 2040.9 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 298 K
$0.40 \times 0.36 \times 0.30$ mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.920, T_{max} = 0.940
18388 measured reflections
4014 independent reflections
2740 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.160
S = 1.04
4014 reflections
239 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1D···O1	0.83	2.58	2.993 (3)	113
N1—H1F···O2	0.78	2.15	2.878 (3)	155
N1—H1F···O3	0.78	2.43	2.990 (3)	129
N1—H1C···O4	0.77	2.12	2.876 (3)	169
N1—H1C···O5	0.77	2.58	3.018 (3)	117
N1—H1D···O6	0.83	2.05	2.871 (3)	172
N1—H1E···F1^i	0.78	2.47	3.179 (4)	151
N1—H1E···F3^i	0.78	2.37	3.080 (3)	152

Symmetry code: (i) $-x + 1, -y + 1, -z$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

References

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supporting information

Ammonium hexafluoridophosphate–18-crown-6 (1/1)

De-Hong Wu and Qi-Qi Wu

S1. Comment

Recently much attention has been devoted to crown ethers due to their ability to form non-covalent, H-bonding complexes with ammonium cations both in solid and in solution (Bajaj *et al.*, 1988; Fender *et al.*, 2002; Kryatova *et al.*, 2004). Both the nature of the ammonium cation (NH_4^+, RNH_3^+, $R_2NH_2^+$, *etc.*) and the size of the crown ether can work on the stability and stoichiometry of these host–guest complexes. The host molecules combine with the guest species by intermolecular interaction, 18-Crown-6 has a high affinity for RNH_3^+ cations and most studies of 18-crown-6 and its derivatives invariably showed a 1:1 stoichiometry with RNH_3^+ cations. For similar structures, see: Dapporto *et al.*, 1996; Pears *et al.*, 1988. In our laboratory, the title compound has been synthesized and its crystal structure is herein reported.

The title compound crystallizes in the $P2_1/n$ space group with an asymmetric unit consisting of a cationic [(NH_4)(18-crown-6)]$^+$ moiety and an isolated anionic PF_6^- (Fig 1). The NH_4^+ nests in the 18-crown-6 ring to form a superamolecular rotator-stator-like structure by intramolecular N—H⋯O hydrogen-bonded interactions between the NH_4^+ (H1C, H1D and H1F) and the six oxygen atoms of the crown ether (Fig 2). Intramolecular N—H⋯O hydrogen distances fall within the normal range: 2.871 (3) and 3.018 (3) Å (Table 1). The six oxygen atoms of the crown ether lie approximately in a plane with the mean deviation of 0.2129 Å, the N atom aparts from the center of the crown ring about 0.864 Å. The slightly distorted tetrahedral cations NH_4^+ further interact with F1^i and F3^i (symmetry code, i: 1 - *x*, 1 - *y*, -*z*) of the slightly distorted octahedral anions PF_6^- (The P—F bond lengths are within the range of 1.51 - 1.60 Å, the F—P—F bond angles are within the range of 87.78 - 92.48°) by intermolecular N—H⋯F hydrogen bonds (Table 1 and Fig 2).

S2. Experimental

In room temperature 18-crown-6 (4 mmol, 1.05 g) were dissolved in 50 ml me thanol, after addition of excess hexa-fluorophosphoric acid to afford a white microcrystallic precipitation for H_3O^+?PF_6^-(18-crown-6) (about 95% yield). Then dissolve the precipitation again in 50 ml water and addition of excess concentrated ammonia to afford the solution without any participation under stirring at the ambient temperature. Block colorless single crystals suitable for X-ray structure analysis were obtained by the slow evaporation of the above solution after a week in air.

The dielectric constant of the compound as a function of temperature indicates that the permittivity is basically temperature-independent (ε = C/(T–T_0)), suggesting that this compound is not ferroelectric or there may be no distinct phase transition occurring within the measured temperature range between 93 K and 433 K (below the compound melting point 463 K).

S3. Refinement

H atoms in the crown ring were placed in calculated positions with C—H = 0.97 Å for Csp^3 atoms, assigned fixed U_{iso} values [U_{iso}(H) = 1.2Ueq(Csp^3)] and allowed to ride. The four H atoms of NH_4^+ were found with N—H bond distances of between 0.7721 and 0.8282 Å in the difference electron density map.
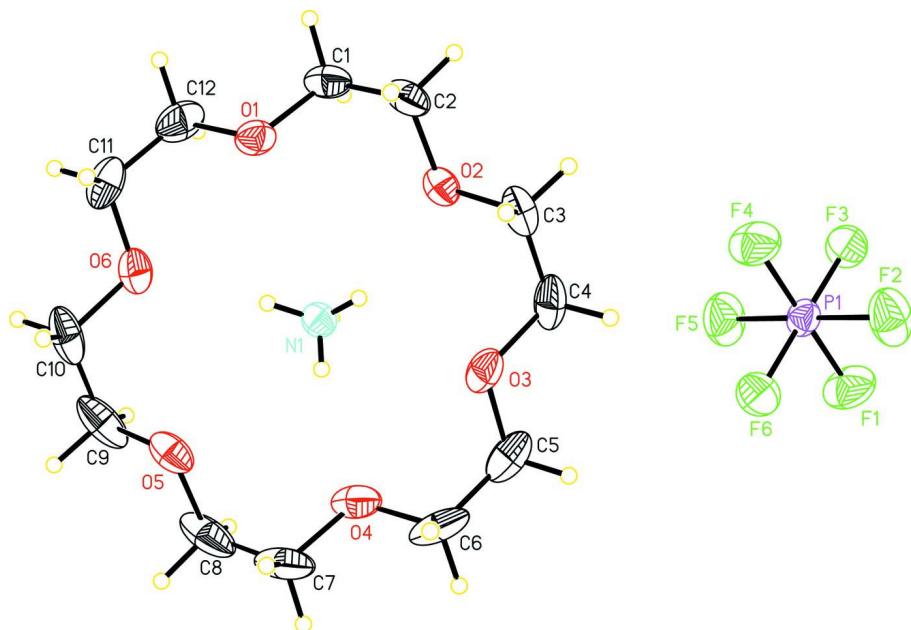
Figure 1

The molecular structure of the title compound, showing the atomic numbering scheme with 30% probability displacement ellipsoids.
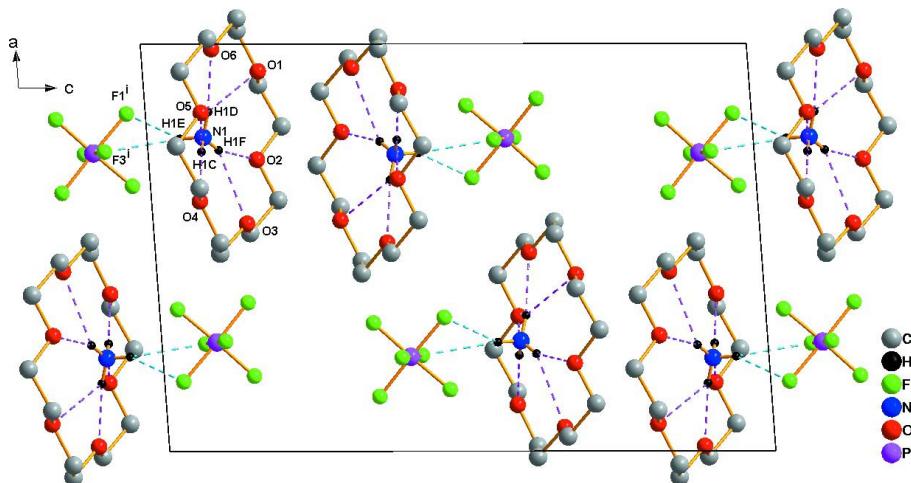
Figure 2

The packing of the title compound viewed along the *b* axis. The i suffix for atoms F1 and F3 denotes a transformation of (1 - *x*, 1 - *y*, -*z*). Hydrogen atoms not involved in hydrogen bonds (dashed lines) are omitted for clarity.

Ammonium hexafluoridophosphate–18-crown-6 (1/1)

Crystal data
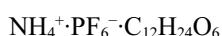
$NH_4^+·PF_6^-·C_{12}H_{24}O_6$	$c = 18.6511 (17)$ Å
$M_r = 427.32$	$β = 94.097 (10)°$
Monoclinic, $P2_1/n$	$V = 2040.9 (7)$ Å³
Hall symbol: -P 2yn	$Z = 4$
$a = 12.559 (3)$ Å	$F(000) = 896$
$b = 8.7352 (17)$ Å	$D_x = 1.391$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 14970 reflections
$\theta = 3.0$–$27.8°$
$\mu = 0.21$ mm^{-1}

$T = 298$ K
Block, colorless
$0.40 \times 0.36 \times 0.30$ mm

Data collection

Rigaku Mercury2
  diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan
  (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.920$, $T_{max} = 0.940$

18388 measured reflections
4014 independent reflections
2740 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 26.0°$, $\theta_{min} = 3.0°$
$h = -15\rightarrow15$
$k = -10\rightarrow10$
$l = -23\rightarrow23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.160$
$S = 1.04$
4014 reflections
239 parameters
0 restraints
Primary atom site location: structure-invariant
  direct methods

Secondary atom site location: difference Fourier
  map
Hydrogen site location: inferred from
  neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 1.0944P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.9000 (3)	0.5093 (4)	0.18932 (18)	0.0655 (9)
H1A	0.9538	0.4465	0.2150	0.079*
H1B	0.8914	0.4736	0.1400	0.079*
C2	0.7979 (3)	0.4959 (3)	0.22323 (17)	0.0642 (9)
H2A	0.7804	0.3888	0.2295	0.077*
H2B	0.8038	0.5441	0.2702	0.077*
C3	0.6165 (3)	0.5644 (4)	0.20892 (18)	0.0660 (9)
H3A	0.6212	0.6175	0.2547	0.079*
H3B	0.5959	0.4592	0.2171	0.079*
C4	0.5360 (3)	0.6394 (4)	0.1589 (2)	0.0739 (10)
H4A	0.5371	0.5935	0.1116	0.089*
H4B	0.4654	0.6249	0.1757	0.089*

C5	0.4855 (3)	0.8783 (5)	0.1069 (2)	0.0886 (12)
H5A	0.4135	0.8634	0.1212	0.106*
H5B	0.4889	0.8384	0.0586	0.106*
C6	0.5118 (3)	1.0437 (5)	0.1080 (2)	0.0931 (14)
H6A	0.4575	1.0999	0.0793	0.112*
H6B	0.5138	1.0819	0.1569	0.112*
C7	0.6458 (4)	1.2199 (4)	0.0808 (2)	0.0938 (15)
H7A	0.6540	1.2563	0.1300	0.113*
H7B	0.5920	1.2822	0.0547	0.113*
C8	0.7494 (5)	1.2330 (4)	0.0468 (2)	0.0967 (16)
H8A	0.7437	1.1844	−0.0001	0.116*
H8B	0.7670	1.3400	0.0403	0.116*
C9	0.9326 (4)	1.1636 (4)	0.0621 (2)	0.0895 (14)
H9A	0.9540	1.2689	0.0549	0.107*
H9B	0.9277	1.1127	0.0158	0.107*
C10	1.0131 (3)	1.0861 (4)	0.1110 (2)	0.0822 (12)
H10A	1.0832	1.0972	0.0928	0.099*
H10B	1.0150	1.1331	0.1582	0.099*
C11	1.0631 (3)	0.8462 (5)	0.1619 (2)	0.0795 (11)
H11A	1.0637	0.8851	0.2106	0.095*
H11B	1.1341	0.8587	0.1453	0.095*
C12	1.0335 (3)	0.6825 (5)	0.1605 (2)	0.0787 (11)
H12A	1.0287	0.6452	0.1114	0.094*
H12B	1.0876	0.6234	0.1880	0.094*
F1	0.17131 (17)	0.4032 (3)	0.03130 (14)	0.1043 (8)
F2	0.18504 (19)	0.3563 (3)	0.14865 (13)	0.1016 (8)
F3	0.26429 (15)	0.2017 (2)	0.07209 (11)	0.0776 (6)
F4	0.36548 (17)	0.3544 (2)	0.14682 (12)	0.0929 (7)
F5	0.34845 (19)	0.4032 (3)	0.02988 (13)	0.1027 (8)
F6	0.27021 (16)	0.5594 (2)	0.10520 (12)	0.0840 (6)
N1	0.7710 (2)	0.8261 (3)	0.09254 (14)	0.0488 (6)
H1C	0.7357	0.8983	0.0882	0.13 (2)*
H1E	0.7676	0.7882	0.0543	0.096 (15)*
H1D	0.8331	0.8534	0.1039	0.113 (16)*
H1F	0.7393	0.7719	0.1167	0.14 (2)*
O1	0.93305 (15)	0.6644 (2)	0.19077 (11)	0.0558 (5)
O2	0.71616 (16)	0.5684 (2)	0.17870 (10)	0.0539 (5)
O3	0.55889 (15)	0.7988 (3)	0.15465 (11)	0.0620 (6)
O4	0.6137 (2)	1.0656 (2)	0.07955 (12)	0.0709 (7)
O5	0.8311 (2)	1.1606 (2)	0.09173 (11)	0.0653 (6)
O6	0.98772 (17)	0.9291 (2)	0.11637 (11)	0.0631 (6)
P1	0.26791 (6)	0.38092 (9)	0.09059 (4)	0.0537 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.080 (2)	0.0483 (18)	0.068 (2)	0.0199 (16)	−0.0022 (18)	0.0009 (15)
C2	0.094 (3)	0.0443 (17)	0.0532 (18)	−0.0058 (17)	−0.0063 (17)	0.0113 (14)

C3	0.076 (2)	0.0564 (19)	0.068 (2)	−0.0250 (17)	0.0198 (18)	−0.0071 (16)
C4	0.056 (2)	0.080 (2)	0.087 (2)	−0.0299 (18)	0.0119 (18)	−0.030 (2)
C5	0.0465 (19)	0.129 (4)	0.087 (3)	0.008 (2)	−0.0148 (18)	−0.012 (3)
C6	0.073 (3)	0.110 (3)	0.092 (3)	0.054 (2)	−0.021 (2)	−0.008 (2)
C7	0.135 (4)	0.049 (2)	0.089 (3)	0.032 (2)	−0.054 (3)	−0.0103 (19)
C8	0.179 (5)	0.045 (2)	0.060 (2)	−0.015 (3)	−0.035 (3)	0.0138 (17)
C9	0.156 (4)	0.049 (2)	0.070 (2)	−0.025 (2)	0.055 (3)	−0.0036 (17)
C10	0.084 (3)	0.070 (2)	0.099 (3)	−0.039 (2)	0.052 (2)	−0.025 (2)
C11	0.0392 (17)	0.115 (3)	0.086 (3)	−0.0054 (19)	0.0125 (17)	−0.009 (2)
C12	0.054 (2)	0.096 (3)	0.088 (3)	0.029 (2)	0.0155 (18)	0.001 (2)
F1	0.0796 (15)	0.1011 (18)	0.1247 (19)	0.0091 (12)	−0.0443 (14)	−0.0083 (14)
F2	0.1082 (17)	0.0858 (15)	0.1183 (18)	−0.0139 (13)	0.0598 (15)	−0.0182 (13)
F3	0.0747 (13)	0.0560 (12)	0.1020 (15)	−0.0021 (9)	0.0051 (11)	−0.0175 (10)
F4	0.0879 (15)	0.0858 (15)	0.0988 (16)	0.0013 (12)	−0.0361 (12)	−0.0043 (12)
F5	0.0939 (16)	0.1138 (19)	0.1056 (17)	−0.0110 (14)	0.0442 (14)	0.0028 (14)
F6	0.0805 (14)	0.0547 (11)	0.1155 (17)	−0.0061 (10)	−0.0009 (12)	−0.0113 (11)
N1	0.0531 (16)	0.0445 (13)	0.0488 (15)	−0.0016 (13)	0.0033 (11)	−0.0026 (12)
O1	0.0524 (12)	0.0529 (12)	0.0626 (13)	0.0132 (9)	0.0082 (10)	0.0004 (10)
O2	0.0625 (13)	0.0496 (11)	0.0503 (11)	−0.0075 (10)	0.0083 (10)	0.0056 (9)
O3	0.0420 (11)	0.0733 (15)	0.0690 (14)	−0.0032 (10)	−0.0083 (10)	−0.0175 (11)
O4	0.0833 (17)	0.0540 (13)	0.0717 (15)	0.0239 (12)	−0.0210 (13)	−0.0119 (11)
O5	0.1022 (18)	0.0461 (12)	0.0478 (12)	−0.0099 (12)	0.0068 (12)	0.0064 (9)
O6	0.0569 (13)	0.0651 (13)	0.0689 (14)	−0.0166 (11)	0.0165 (11)	−0.0052 (11)
P1	0.0441 (4)	0.0524 (5)	0.0643 (5)	−0.0032 (4)	0.0011 (3)	−0.0086 (4)

Geometric parameters (Å, º)

C1—O1	1.416 (4)	C8—H8A	0.9700
C1—C2	1.475 (5)	C8—H8B	0.9700
C1—H1A	0.9700	C9—O5	1.424 (5)
C1—H1B	0.9700	C9—C10	1.477 (6)
C2—O2	1.422 (4)	C9—H9A	0.9700
C2—H2A	0.9700	C9—H9B	0.9700
C2—H2B	0.9700	C10—O6	1.413 (4)
C3—O2	1.410 (4)	C10—H10A	0.9700
C3—C4	1.478 (5)	C10—H10B	0.9700
C3—H3A	0.9700	C11—O6	1.423 (4)
C3—H3B	0.9700	C11—C12	1.478 (5)
C4—O3	1.425 (4)	C11—H11A	0.9700
C4—H4A	0.9700	C11—H11B	0.9700
C4—H4B	0.9700	C12—O1	1.426 (4)
C5—O3	1.417 (4)	C12—H12A	0.9700
C5—C6	1.482 (6)	C12—H12B	0.9700
C5—H5A	0.9700	F1—P1	1.594 (2)
C5—H5B	0.9700	F2—P1	1.569 (2)
C6—O4	1.432 (5)	F3—P1	1.6029 (19)
C6—H6A	0.9700	F4—P1	1.572 (2)
C6—H6B	0.9700	F5—P1	1.583 (2)

C7—O4	1.407 (4)	F6—P1	1.583 (2)
C7—C8	1.492 (6)	N1—H1C	0.7721
C7—H7A	0.9700	N1—H1E	0.7840
C7—H7B	0.9700	N1—H1D	0.8282
C8—O5	1.427 (5)	N1—H1F	0.7827
O1—C1—C2	109.3 (2)	C10—C9—H9A	109.6
O1—C1—H1A	109.8	O5—C9—H9B	109.6
C2—C1—H1A	109.8	C10—C9—H9B	109.6
O1—C1—H1B	109.8	H9A—C9—H9B	108.1
C2—C1—H1B	109.8	O6—C10—C9	109.9 (3)
H1A—C1—H1B	108.3	O6—C10—H10A	109.7
O2—C2—C1	109.1 (2)	C9—C10—H10A	109.7
O2—C2—H2A	109.9	O6—C10—H10B	109.7
C1—C2—H2A	109.9	C9—C10—H10B	109.7
O2—C2—H2B	109.9	H10A—C10—H10B	108.2
C1—C2—H2B	109.9	O6—C11—C12	109.0 (3)
H2A—C2—H2B	108.3	O6—C11—H11A	109.9
O2—C3—C4	108.9 (3)	C12—C11—H11A	109.9
O2—C3—H3A	109.9	O6—C11—H11B	109.9
C4—C3—H3A	109.9	C12—C11—H11B	109.9
O2—C3—H3B	109.9	H11A—C11—H11B	108.3
C4—C3—H3B	109.9	O1—C12—C11	109.2 (3)
H3A—C3—H3B	108.3	O1—C12—H12A	109.8
O3—C4—C3	109.7 (2)	C11—C12—H12A	109.8
O3—C4—H4A	109.7	O1—C12—H12B	109.8
C3—C4—H4A	109.7	C11—C12—H12B	109.8
O3—C4—H4B	109.7	H12A—C12—H12B	108.3
C3—C4—H4B	109.7	H1C—N1—H1E	104.9
H4A—C4—H4B	108.2	H1C—N1—H1D	108.4
O3—C5—C6	109.5 (3)	H1E—N1—H1D	110.2
O3—C5—H5A	109.8	H1C—N1—H1F	104.0
C6—C5—H5A	109.8	H1E—N1—H1F	105.7
O3—C5—H5B	109.8	H1D—N1—H1F	122.3
C6—C5—H5B	109.8	C1—O1—C12	111.4 (2)
H5A—C5—H5B	108.2	C3—O2—C2	112.3 (2)
O4—C6—C5	109.3 (3)	C5—O3—C4	112.9 (3)
O4—C6—H6A	109.8	C7—O4—C6	112.6 (3)
C5—C6—H6A	109.8	C9—O5—C8	112.9 (3)
O4—C6—H6B	109.8	C10—O6—C11	113.1 (3)
C5—C6—H6B	109.8	F2—P1—F4	92.48 (14)
H6A—C6—H6B	108.3	F2—P1—F6	91.19 (12)
O4—C7—C8	108.9 (3)	F4—P1—F6	91.52 (12)
O4—C7—H7A	109.9	F2—P1—F5	177.92 (14)
C8—C7—H7A	109.9	F4—P1—F5	89.31 (14)
O4—C7—H7B	109.9	F6—P1—F5	89.83 (13)
C8—C7—H7B	109.9	F2—P1—F1	89.19 (15)
H7A—C7—H7B	108.3	F4—P1—F1	177.60 (14)

O5—C8—C7	109.2 (3)	F6—P1—F1	90.16 (12)
O5—C8—H8A	109.8	F5—P1—F1	88.99 (15)
C7—C8—H8A	109.8	F2—P1—F3	90.29 (11)
O5—C8—H8B	109.8	F4—P1—F3	90.49 (11)
C7—C8—H8B	109.8	F6—P1—F3	177.45 (13)
H8A—C8—H8B	108.3	F5—P1—F3	88.63 (12)
O5—C9—C10	110.1 (3)	F1—P1—F3	87.78 (12)
O5—C9—H9A	109.6		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1D···O1	0.83	2.58	2.993 (3)	113
N1—H1F···O2	0.78	2.15	2.878 (3)	155
N1—H1F···O3	0.78	2.43	2.990 (3)	129
N1—H1C···O4	0.77	2.12	2.876 (3)	169
N1—H1C···O5	0.77	2.58	3.018 (3)	117
N1—H1D···O6	0.83	2.05	2.871 (3)	172
N1—H1E···F1[i]	0.78	2.47	3.179 (4)	151
N1—H1E···F3[i]	0.78	2.37	3.080 (3)	152

Symmetry code: (i) $-x+1, -y+1, -z$.